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The main goal of this work has been the development, measurement, and understanding of quantum dot qubits in silicon/silicon-germanium. Our team has approached this goal from both experimental and theoretical perspectives, covering materials, coherence, qubit fabrication, and measurement. Achievements include the measurement of stable, low noise Coulomb Blockade in a two-dimensional electron gas-based Si/SiGe quantum dot, measurement of spin coherence in silicon quantum wells, development of new schemes for spin measurement and robust quantum gates, measurement of valley states and the low-energy spectrum in Si/SiGe quantum wells, and theoretical understanding of several decoherence mechanisms.

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(1) Forward

The main goal of this work has been the development, measurement, and understanding of quantum dot qubits in silicon/silicon-germanium. Our team has approached this goal from both experimental and theoretical perspectives, covering materials, coherence, qubit fabrication, and measurement. Achievements include the measurement of stable, low noise Coulomb Blockade in a two-dimensional electron gas-based Si/SiGe quantum dot, measurement of spin coherence in silicon quantum wells, development of new schemes for spin measurement and robust quantum gates, measurement of valley states and the low-energy spectrum in Si/SiGe quantum wells, and theoretical understanding of several decoherence mechanisms.

(2) Table of Contents

(3) List of Appendices, Illustrations, and Tables

(4) Statement of the Problem Studied

The challenge this work has addressed is the development of qubits in silicon/silicon-germanium. This is an important goal because of (i) the practical utility of silicon and its established infrastructure and (ii) the fundamental coherence advantages of working with electrons in silicon, a material with a zero spin nuclear isotope, ^{28}Si, and with low spin orbit coupling. The challenge we have addressed is the fabrication and measurement of quantum dots in Si/SiGe, the measurement of spin coherence in silicon quantum wells, the measurement of valley splitting in silicon quantum wells, the development silicon quantum well growth technology, the theoretical understanding of these issues, and the development of new schemes for scalable quantum information processing with silicon-based quantum dot qubits.

(5) Summary of the most important Results

The following results are discussed below:

1. Experimental Si/SiGe heterostructure growth and measurement (performed at IBM and University of Wisconsin-Madison).
2. Experimental measurement of low noise silicon/silicon-germanium quantum dots.
3. A new proposal for readout.
4. Valley splitting in silicon quantum wells.
5. Theory of spin decoherence and impurity effects in quantum dots.
6. Experimental measurements of ESR in silicon dots and two-dimensional electron gases.
7. Simulations of 4 coupled qubits
8. Pseudo-Digital Qubits
9. Spectroscopy of valley splitting in silicon

1. Silicon/Silicon-Germanium Heterostructure Growth and Measurement

Over the past three years, there has been a strong and sustained emphasis on heterostructure growth and characterization. Numerous CVD growth runs were performed at Wisconsin, with the goal of optimizing 2DEG characteristics. The samples were carefully characterized and analyzed, with results fed back into new growth runs. Two different parts of the heterostructure were targeted for improvement. First, we improved the composition grading to efficiently relax the SiGe alloy, grown on a Si substrate. A number of these growths were performed with isotopically purified ^{28}Si. Initial experiments graded the Ge composition in 5% steps of 500 nm thickness. This grading was too discrete, and reducing the grading steps to 2.5% per 250nm yielded samples with improved mobility, up to 90,000 cm^2/Vs at low temperature. This improvement was presumably due to a lower threading-dislocation density. We also examined details of the well thickness, modulation dopant concentration, and doping offset. Doping concentration and offset had the greatest effect, and we are currently optimizing these parameters. The result of this work is that we are now growing Si/SiGe 2DEGs at Wisconsin with mobilities at the same order as our original samples obtained from IBM. Several alternative paths were pursued, to improve strain relaxation of the SiGe effective substrate, while minimizing dislocations. These included growths on oxide substrates (both SOI and SGOI). To date, quantum wells with 2DEG have been achieved. The oxide growth is still in progress and shows tremendous potential for strain management. In addition to these growth advances at Wisconsin, we continue to have strong and productive collaborations with IBM. Very recent IBM samples measured at Wisconsin have shown world-class mobilities greater than 130,000 cm^2/Vs at 2K. In all, over 30 samples have been fully characterized, and many more than that have been grown and partially characterized to address specific questions.

2. Experimental measurement of low noise silicon/silicon-germanium quantum dots.

We have fabricated several generations of quantum dots and double dots in silicon/silicon-germanium (Si/SiGe) heterostructures that show repeatable Coulomb blockade effects. The primary challenge for such structures is the fabrication of highly isolated gates that do not leak current into the active 2DEG. We have overcome this problem by fabricating a dot with highly isolated *side* gates formed by etching the 2DEG itself. As an alternative strategy, we have made considerable progress in fabricating Schottky gates on our 2DEG, deposited on top an intervening layer of oxide deposited by atomic layer deposition (ALD). The latter work represents a collaboration with Cambridge Nanotechnologies, from whom we have recently purchased an ALD machine. In ongoing work, we expect the combination of etching, side-gates, ALD and metal top-gates to provide a rich and productive environment for device fabrication. Below, we describe our results on side-gated single dots.

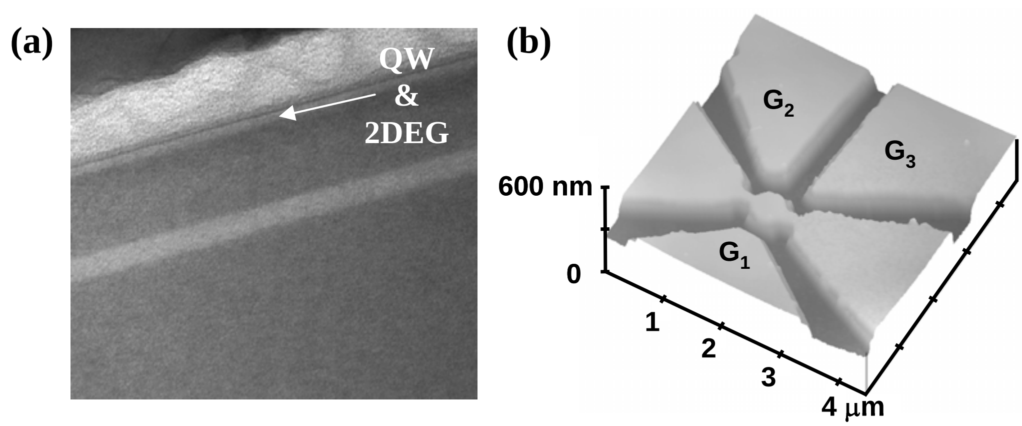

Figure 1: (a) Transmission electron microscope image of the SiGe heterostructure used in this work. The 2DEG sits near the top of the silicon quantum well. (b) Atomic force microscope image of the fabricated dot with three etch-defined electrostatic side gates.

The Si/SiGe heterostructure in Fig. 1(a) was grown at IBM by ultra-high vacuum chemical vapor deposition. The 2DEG sits near the top of 80 Å of strained Si grown on a strain-relaxed $Si_{0.7}Ge_{0.3}$ buffer layer. The 2DEG is separated from the donors by a 140 Å $Si_{0.7}Ge_{0.3}$ spacer layer, and the phosphorus donors lie in a 140 Å $Si_{0.7}Ge_{0.3}$ layer capped with 35 Å of Si at the surface. The electron density in the 2DEG is $4x10^{11}$ cm^{-2} and the mobility is 40,000 cm^2/Vs at 2K.

We fabricated quantum dots by electron beam lithography and subsequent CF_4 reactive-ion etching. Fig. 1(b) shows an atomic force microscope image of the completed structure. Control of the dot electron population and the lead resistances is achieved with three separately tunable gates. Each gate is fabricated from the same 2DEG from which the quantum dot is created.

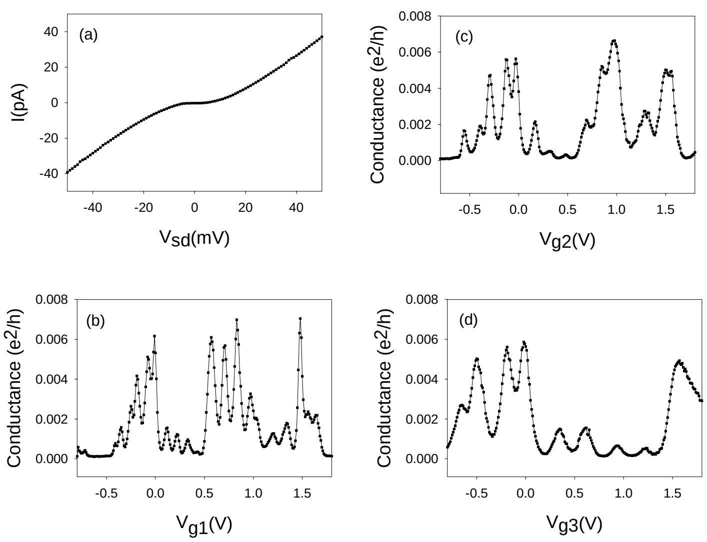

Figure 2: (a) I-V curve through the dot at zero gate bias showing zero conductance up to 4 mV source-drain voltage. (b)-(d) Coulomb blockade oscillations through the quantum dot as the voltage is varied on each of the three side gates (G_1, G_2, G_3) respectively.

A current-voltage (I-V_{ds}) measurement of the dot at zero gate bias taken at 250 mK is shown in Figure 2(a). The leads of the dot are intrinsically pinched off in the tunneling regime, due to surface depletion, such that the Coulomb blockade region is evident at zero gate voltage for $|V_{ds}| < 4$ mV. The dot remains in the tunneling regime up to + 5V applied to the side gates. Conductance oscillations with varying gate voltage are observed for each of the three gates. Typical results are shown in Figure 2(b-d) at 1.8 K. These curves show nicely repeatable Coulomb Blockade. A remaining challenge is that not all of the Coulomb blockade minima reach zero conductance. It may not be necessary for all the minima to reach zero in order to obtain good qubit operation, as an operating point may be chosen. Nonetheless, it remains a goal to increase the number of minima that reach zero conductance.

Figure 3 is a two-dimensional plot showing dI/dV measurements with varying gate and drain-source voltages (Coulomb diamonds) for a more recent quantum dot fabricated at Wisconsin. Here, the Coulomb diamonds show no switching events during the data acquisition period. This is a significant improvement over our previous results, which typically showed several switching events in such a plot. The quantum dot that produced this data is very similar to that shown in Fig. 1 above. The two differences were the following: (a) the dot was annealed in forming gas prior to measurement, and (b) the dot was measured at low temperature for an extended time period. It is not clear yet whether both these changes are critical to observing low charge noise, or whether one or the other had the dominant effect.

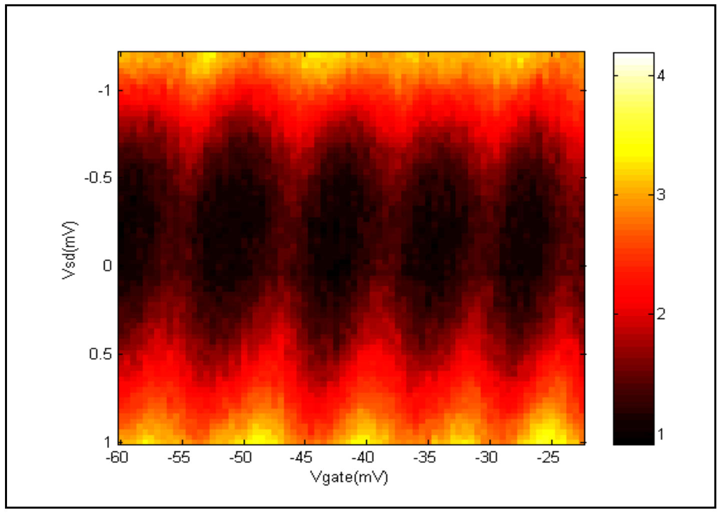

Fig. 3. Coulomb diamond stability plot for second generation Si/SiGe quantum dots fabricated at University of Wisconsin-Madison. No switching events are observed in a scan acquired over a 6 hour time period.

The charging energy to overcome the Coulomb blockade and add an electron to a dot can be estimated from the Coulomb diamond plot. For the dot in Fig. 1, the result is 3.2 meV. The total capacitance of the dot as calculated from the charging energy is 50 aF. This corresponds to a disk of diameter 120 nm in an infinite dielectric. We can make a better estimate with Poisson simulations of the full device, using an adaptive finite element mesh, and treating 2DEG regions (dot, leads, and gates) with fixed-voltage boundary conditions. We thus estimate an electronic dot diameter of D = 233 nm. This result compares favorably to independent measurements of ~200 nm surface depletion in quantum wires of variable width that were fabricated in a similar manner. From the electronic dot diameter and the sheet density of electrons in the original 2DEG, we estimate that there are ~170 electrons in the dot under the operating conditions of Fig. 2. Fabrication of smaller dots using the etch-defined gates described here will allow lower electron occupation of the dot. It is likely that achievement of individual electron quantum dots will require either etch-defined gates that are more closely coupled than those demonstrated here, or the use of metal top gates to confine the electrons laterally. We note that the simulations used to extract the dot size are an example of closing the loop between theory, simulation, and experiment, one of the goals that came out of our site visit in spring, 2003.

3. Proposal for readout

The final step of a quantum computation is to read out the spins of the qubit register. However, the qubits must also be measured and re-initialized regularly during the computation, in the context of fault-tolerant quantum error correction. Fast readout is therefore a requisite for scalable quantum computing. Unfortunately, the main advantage of spin qubits (their weak coupling to the environment) makes fast measurement a challenge. The original proposals for solid-state spin quantum computers by Kane and Loss and DiVincenzo suggest using the Pauli principle to convert spin information to a charge signal, which is more readily detected. Recent advancements in radio-frequency single-electron transistors (rf-SETs) make it possible to detect single electrons with very high bandwidth.

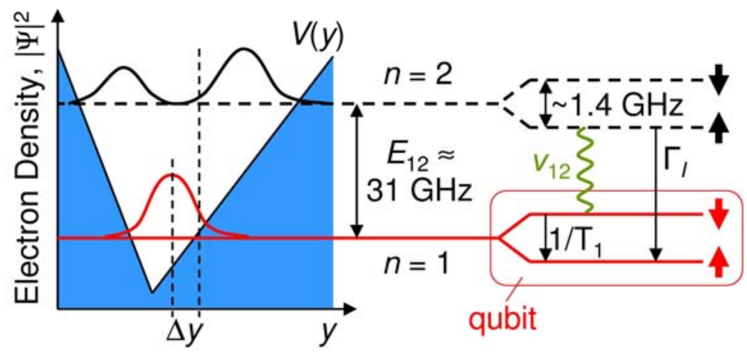

Fig. 4. Energy spectrum of the proposed readout dot. The orbital ground state (n = 1) defines the qubit. Microwaves of energy v_{12} can excite the electron from $|1\downarrow\rangle$ to $|2\uparrow\rangle$. Because of the asymmetric confinement potential $V(y)$, the orbital excitation is accompanied by center of mass motion Δy, which can be detected by a nearby charge sensor.

At present, fast single spin detection in quantum dots remains elusive, although tantalizing preliminary results have recently been reported by the Kouwenhoven/vanderSypen collaboration. Such promising schemes rely on ancillary tunnel couplings, which may provide unwanted channels for decoherence. To address the problem of fast, scalable readout, we proposed a microwave-based scheme to enable spin-charge transduction within a single dot [PRL **92**, 037901 (2004)]. The same quantum dot can be used for rapid initialization, gating and readout. The scheme works as follows. As shown in Fig. 4, a qubit electron can be promoted from its ground state to an excited state by applying microwaves of energy $v_{12} = E_2 - E_1$. In a magnetic field, this process becomes spin dependent if the microwave field connects states of opposite spin. For spins originally in the "down" state $|1\downarrow\rangle$, the microwaves cause Rabi oscillations into the excited orbital $|2\uparrow\rangle$. Although this transition involves a spin flip, which is classically forbidden by electric dipole selection rules, it may still take place in semiconductor quantum dots because of spin-orbit coupling, which mixes the pure spin eigenstates. To read out the spin, the orbital oscillations are transformed into charge oscillations by creating a quantum dot confinement potential that is slightly asymmetric. The excited orbital will then have a center of mass that is shifted from the ground state. By integrating an rf-SET into the device, as shown in Fig. 5, the charge motion (and thus the original spin state) can be detected. The stronger the capacitive coupling between the SET island and the quantum dot, the faster the measurement. We also note that the excited electronic orbital decays rather quickly to the ground state. We can utilize this process for initialization, since the decay occurs without a spin flip, with very high probability.

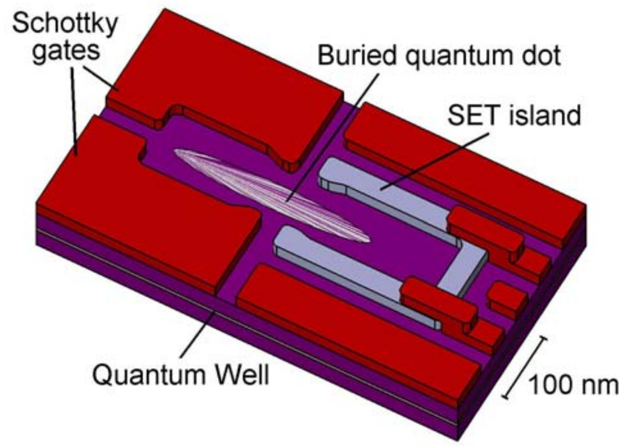

Fig. 5 One of the many devices simulated in this work. Note the strong capacitive coupling between the SET island and the quantum dot.

We have investigated the feasibility of our proposed readout device by using both analytical theory and simulations. The results, reported in our PRL, allow us to (i) navigate the enormous parameter space for this device, (ii) determine the coupling strength between the quantum dot and the rf-SET, and thus the sensitivity of readout, (iii) calculate the rates for orbital excitation and decay, which, combined with the rf-SET specifications, allow us to determine whether the experiment will succeed. Our calculations show that excitation and decay rates depend sensitively on materials and device properties. Although challenging, we believe fast spin readout and initialization is possible.

4. Valley splitting in silicon quantum wells.

The implementation of spin qubits in quantum dots assumes that the only quantum mechanical degree of freedom available to the qubits lies in the spin sector. Resonant excitation of the electron into any nearby electronic or orbital states forms a source of "leakage" outside the qubit Hilbert space. If uncontrolled, this leakage can be viewed as decoherence. It is therefore crucial that the ground orbital/electronic state of the quantum dot is non-degenerate. In the absence of strain, the conduction-band minimum in silicon is six-fold degenerate. Strain in Si/SiGe heterostructures reduces the degeneracy to two-fold. The remaining degeneracy is broken by the strong vertical confinement of the qubit electron inside the quantum well. In a recent paper [APL **84**, 115 (2004)] and preprint [submitted to PRB], we have quantified this valley splitting, showing that leakage is not a threat to silicon-based qubits.

The sharp boundaries of the quantum well barriers make this problem unsuitable for study using conventional effective mass techniques. Indeed, existing theoretical treatments of such heterostructures invoke phenomenological and poorly understood parameters to describe the interference between the two degenerate valleys. We have therefore approached the problem from the more fundamental perspective of tight-binding theory, with no phenomenological parameters. Two separate methods were used: (i) a simple but powerful 2-band model enabled analytical results, while (ii) highly accurate, quantitative results were obtained using the nano-electronic modeling software NEMO. The simpler model, while utilizing many fewer energy bands than NEMO, achieves impressive qualitative and quantitative accuracy, and can be regarded as a theoretical breakthrough for the treatment of silicon quantum wells. Both the analytical and computational efforts were performed in collaboration with Gerhard Klimeck at Purdue (formerly at JPL).

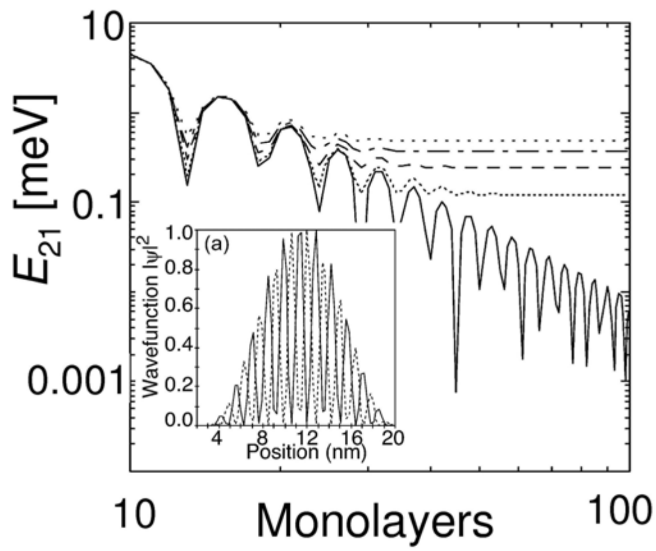

Fig. 6. Computed valley splitting E_{21} vs number of atomic monolayers in the quantum well. Solid line corresponds to zero applied field; oscillations reflect transitions of valley ground state from even to odd symmetry. Dotted and dashed lines correspond to finite applied E fields between 1-4 mV/nm. Inset: even and odd symmetry traces of tight-binding coefficients for a pair of valley split ground states.

The main results of our investigation are shown in Fig. 6. We see that the valley splitting E_{12} can be engineered by varying the well width, or by applying a vertical electric field. Indeed, strong internal electric fields of order 6 mV/nm occur naturally in such modulation doped structures. Our quantitative calculations indicate that valley splittings greater than 1 meV can be obtained in such environments. Thus, thermal excitation of higher valley states can be avoided by operating our quantum dots at temperatures far below 10 K. And non-adiabatic excitation can be avoided by employing gate times much longer than 4 ps. Both of these conditions are extremely reasonable for a silicon quantum computing as currently envisioned. (Section 9 below contains details on experimental measurement of valley splitting.)

5. Theory of spin decoherence and impurity effects in quantum dots

In the past year we continued our investigation of decoherence mechanisms important for our proposed silicon qubits. Several new and significant mechanisms were identified, including electrostatic and exchange coupling between qubits and impurities, spin-flip scattering in Si quantum dots due to Rashba spin-orbit coupling, and decay of orbital and valley excited states. We have performed a full analysis of decoherence arising from Rashba coupling in 2DEG structures. We describe each of these separate results briefly below.

Impurity effects. Impurities will have a detrimental effect on quantum computing in quantum dots. We have quantified the interactions between impurities and qubits, and considered their implications for scalability. For remote charged states, such as surface states or ionized dopants in the supply layer, the impurities can scatter mobile electrons in the 2DEG, causing a decrease in mobility, or affecting the electrostatic definition and control of quantum dot gate operations. Although such effects are serious, they can usually be compensated in well-characterized qubits. However, from the standpoint of decoherence and scalability, *neutral* dopant impurities like P in Si pose a more serious problem. Such donor-bound spins are abundant in the supply layer, but they also occur at low densities throughout the sample. These impurities can potentially act as parasitic qubits, siphoning off quantum information in an uncontrolled way. When the exchange coupling between the impurity and a qubit becomes large enough, fault-tolerant quantum error correction schemes are no longer effective.

To investigate this issue, we have computed the qubit-impurity exchange coupling J for two cases: (i) impurities in the supply layer, and (ii) impurities in or near the quantum well. In the first case, due to the potentially large numbers of neutral donors in the supply layer, the important parameter for our calculation is the distance between the supply layer and the quantum well. We have determined a minimum safe set-back distance of 8 nm between the quantum well and P dopants in the supply layer. This result depends only weakly on the heterostructure geometry or on the choice of fault-tolerance schemes and error correction coding, due to the exponential dependence of the exchange coupling on qubit-impurity separation. However, the results depend sensitively on the choice of barrier materials and, in particular, on the height of the quantum well barriers. Fortunately, the safe set-back distance is consistent with a typical modulation doping set-back of approximately 10 nm in Si.

We have also studied the effect of dilute, random impurities in or near the quantum well. We find that electron spins trapped on P impurities within the quantum well pose a threat to qubits at a distances less than 60 nm. The results are somewhat sensitive to the specific details of the qubit confinement potential. A crucial observation, from the perspective of scalability, is that the computed impurity danger zones are approximately equal to the radius of a single electron dot. That is, a single impurity can kill (at most) one or two qubits in a 1D array. Therefore, a modest amount of parallel connectivity would enable scalability, as long as the impurity density is somewhat smaller than the qubit density. For random, dilute P:Si impurities, we estimate the critical density as 1.6×10^{16} cm^{-3} (assuming a 6 nm quantum well). Such purity levels are easily achievable in good materials.

Rashba spin-orbit coupling in silicon. Typical SiGe heterostructures are very asymmetric in the growth direction. This asymmetry leads to the so-called Rashba spin-orbit coupling in silicon quantum wells. We have developed a *k.p* energy-band theory to calculate the zero-magnetic field conduction band spin-splitting due to this effect. Our results for typical, state-of-the-art devices give a Rashba coefficient of $\alpha_R = 1-6$ m/s which corresponds to a spin-splitting of roughly 1 μeV, at least 1000 times smaller than the number for GaAs. Our theory is applicable to many silicon devices in strong electric fields, and the results have implications for both "classical" spintronics and quantum spin-based devices.

Qubit spin-flip time, T_1. Understanding spin-orbit coupling in silicon nanostructures has led to accurate calculations of the T_1 spin-flip times in gated single electron Si quantum dots. This energy relaxation mechanism sets the upper bound on coherence times in spin-based qubit systems. Indeed, in certain situations T_1 is of the same order as T_2, the quantum coherence time, making an accurate knowledge of T_1 very important. We find the following expression for T_1 in silicon quantum dots: $\frac{1}{T_1} \sim \alpha^2 \frac{B^7}{(\hbar\omega_0)^4}$, suggesting that the physical dimension of the dot, $L \sim (\hbar\omega_0)^{-1/2}$, should have a very strong affect on relaxation times. Our result differs both from previous results on donor-bound qubits in silicon and from quantum dot implementations in GaAs.

Orbital decay during readout. We have calculated the orbital decay times relevant for the readout/initialization scheme described above. Specifically, we have obtained the relaxation and optical transition rates of the electron while it is in the excited orbital used for spin-charge transduction.

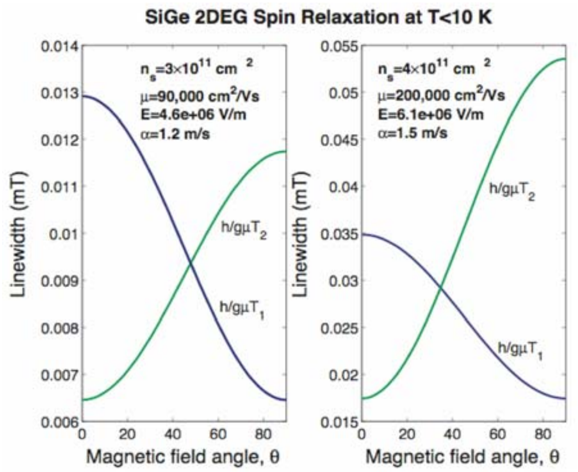

Fig. 7. ESR linewidths calculated for two different 2DEGs, with specifications as shown.

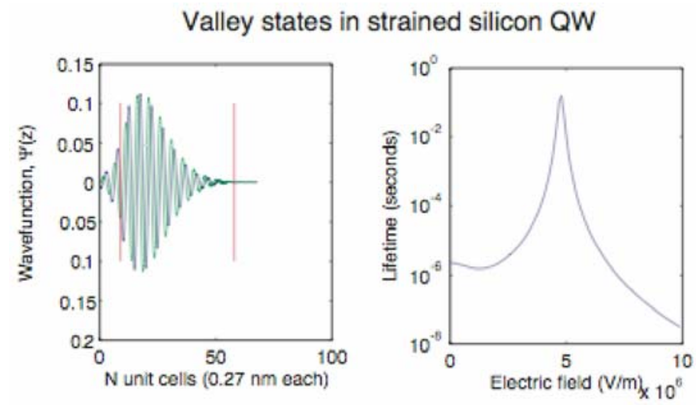

Fig. 8. Decay of valley states. Left: wavefunction in a quantum well in the presence of a strong *E* field, obtained using the tight-binding method. Right: calculated lifetimes of excited valley states.

Spin relaxation in a 2DEG. We have calculated the spin relaxation times of two-dimensional electron gases in SiGe quantum wells. A standalone result in itself, this also has great relevance to the experimental quantum dot ESR measurement roadmap at Wisconsin-Madison. We find that relaxation times increase in the high-mobility limit, as shown in Fig. 7.

Decay of valley states. Going beyond the valley splitting analysis above, we have recently considered how valley states could be harnessed as a potentially useful resource for silicon quantum computing. The valley states are unique to silicon and may have important signatures in transport and ESR experiments. Like other electronic excitations, the valley states can decay to their ground state, as shown in Fig. 8.

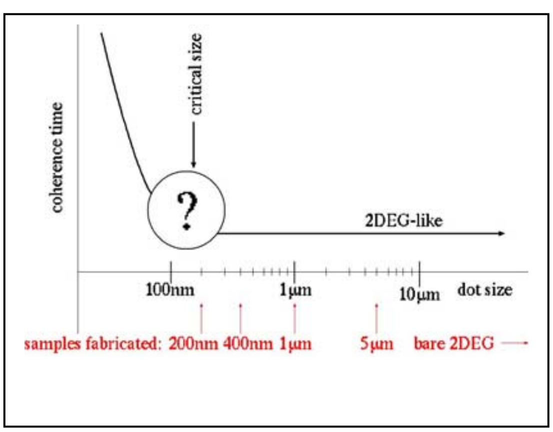

Fig. 9. Schematic of expectation for coherence time dependence as a function of lateral confinement. At a critical size, the electron states will be begin to become localized, at which point momentum scattering will no longer be a source of decoherence, and the coherence time is expected to increase. An approximation for this critical size can be made by equating the energy level spacing for a finite square well with a thermal energy of 4-10K, leading to a well width of 100-250nm.

6. ESR Measurements of Si/SiGe 2DEGs and Dots

The spin coherence of electrons in Si/SiGe quantum wells has been measured to be as large as a few microseconds. However, it is anticipated that the source of decoherence for that system is strongly dependent on electron momentum scattering, implying that electrons in quantum dots should have much longer coherence times (Fig. 9). In the case of very lightly doped phosphorus donors in silicon (a system with many similarities to quantum dots), coherence times have been measured to be 1ms, with an extrapolation up to 62ms [Tyryshkin et. al, PRB 68, 193207 (2003)]. Here, we report our progress in extending this type of analysis to quantum dots.

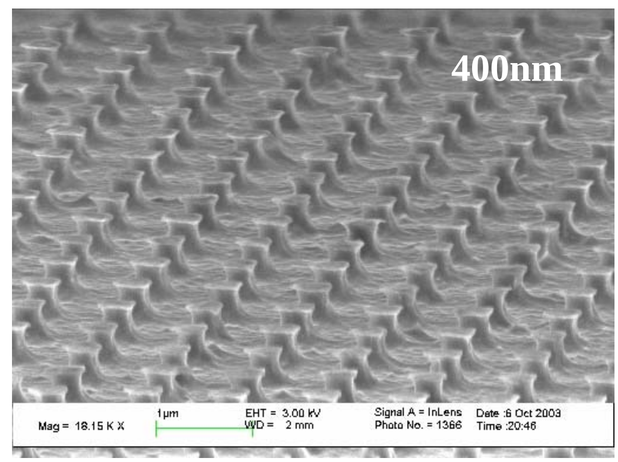

Fig. 10. Scanning Electron Micrograph of an example of the dot arrays etched into a Si/SiGe 2DEG. The dot width for this sample is roughly 400nm, and the etch is around 180nm deep.

In order to measure the spin coherence of electrons in quantum dots, we have created large arrays of dots with sizes ranging from 200 nanometers to 5 micrometers, using electron beam lithography (Fig. 10). The dots were etched with an SF6 reactive ion etch, and cleaned with a RCA organics clean and HF dip.

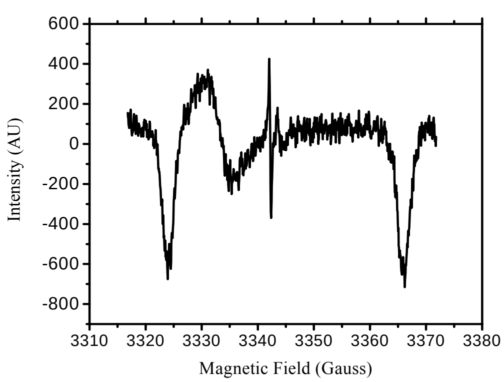

Fig. 11. The sharp central line is the ESR response from a Si/SiGe 2DEG. Dot signals are similar.

Very large numbers of dots were created, so that there would be enough dots to produce a good ESR signal. The fabrication of such large arrays required several modifications to the usual electron beam lithography procedures. Continuous wave electron spin resonance experiments were performed at 4.2K on these dot arrays using a Bruker ESP300E spectrometer and Oxford Instruments ESR continuous flow cryostat. We were able to obtain ESR signals on both unpatterned 2DEGs and on

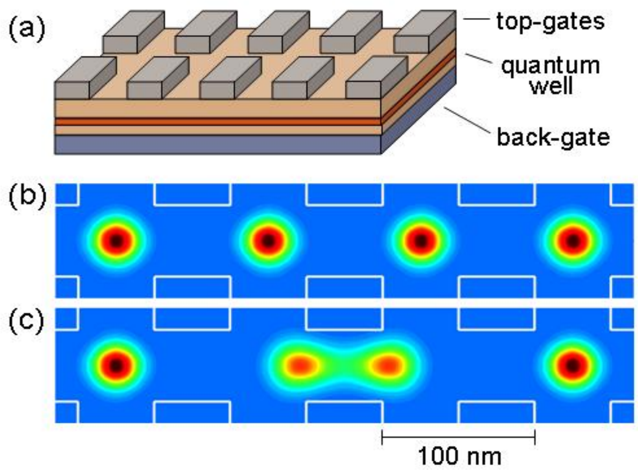

Figure 12. (a) The simulated four-qubit device, including lithographically patterned metallic top-gates, a SiGe quantum well and barriers, an n^+-doped SiGe back-gate. **(b)** Computed charge densities in the quantum well (top-view), with the outlines of metal gates shown in white. All quantum barriers are set "high". **(c)** In this case, the central barrier is lowered, to initiate exchange interaction.

all of the dot sizes fabricated so far, down to 200 nm physical dimensions. (Note that the size of electron confinement inside the dots will be somewhat less than its physical dimensions, due to depletion effects on the etched sides.) Inhomogeneous effects seem to be important in these dots, so further study is planned using pulsed ESR in collaboration with S. Lyon, Princeton University.

7. Simulations of 4 Coupled Qubits

A main focus of the strong collaboration between theory and experiment at Wisconsin has been to adapt the proposed schemes for quantum dot qubits to silicon technology, and to establish or optimize the feasibility of silicon-based devices. Thus, we have established a significant program to develop software for detailed, self-consistent device modeling, with the goal of obtaining feasibility estimates that are as realistic as possible, using state-of-the-art technology. The code combines Poisson and Schroedinger finite-element techniques self-consistently. We have performed simulations of one to four coupled qubits, including qubits for readout and other functionality. We have also initiated collaborations with the Klimeck/NEMO group, to include atomistic effects like valley splitting, which go beyond the effective mass approximations incorporated into our computational models. Below, we describe the results of a simulation performed at Wisconsin for four coupled dots, to answer the question of whether gate operations on specific qubits will adversely affect neighboring qubits.

The four-qubit device is shown in Fig. 12 (a). Fig. 12 (b) shows the computed charge densities when all inter-qubit couplings are extinguished. For realistic gate voltages, the exchange couplings between neighbor qubits in this "off" configuration are found to be $J \approx 10^{-19}$ eV. In the "on" configuration shown in Fig. 12(c), the exchange coupling between two of the four qubits is increased to $J \approx 0.4$ μeV, allowing a two-qubit SWAP gate to be completed in 5 nsec. At the same time, the two outer qubits experience negligible changes in their couplings. Assuming lithographic feature sizes of 30 nm, consistent with our new lithography capabilities, it is possible to perform SWAP gates at speeds much less than 5 nsec. We have verified that our qubits should remain stable against electrons tunneling into or out of their quantum dots, even as top-gate voltages are varied during gate operation. All simulations reported here take into account the full 3-dimensional complexity of the device electrostatics and provide an essentially exact solution for the low-lying energy states.

8. Pseudo-Digital Qubits

As described in the theory section of the QIST roadmap, a crucial role for theory efforts is the development of scalable architectures for specific physical implementations. We have considered not only the scalability of our proposed silicon qubits, but also the peripheral, non-quantum technologies, such as control electronics. The simulations described in this section were used to determine the specifications for such electronics, and to determine the feasibility of an improved qubit architecture, designed to enhance gate control.

Our previous simulations provide estimates for the speed of gates based on the exchange interaction. Typically, such gates will be performed at or near maximum speed, in order to outpace decoherence. However, voltage pulses needed for fast operation are generated by classical, analog circuitry. Thus, pulse shapes will be slightly imperfect, allowing significant errors to accumulate during gating. Taking into account threshold theorems for fault-tolerant computing, and specifications for state-of-the-art pulse generators (e.g. Agilent 8133A), we estimate that conventional qubit architectures, like Fig. 12 (a), cannot possibly support large-scale quantum computing in SiGe. The situation is even worse for GaAs-based schemes due to much shorter coherence times. To improve this situation, we have proposed the "pseudo-digital exchange architecture" shown in Fig. 13 (a). Rather than initiating an exchange coupling by lowering the potential barrier between two qubits, causing the electrons to slide

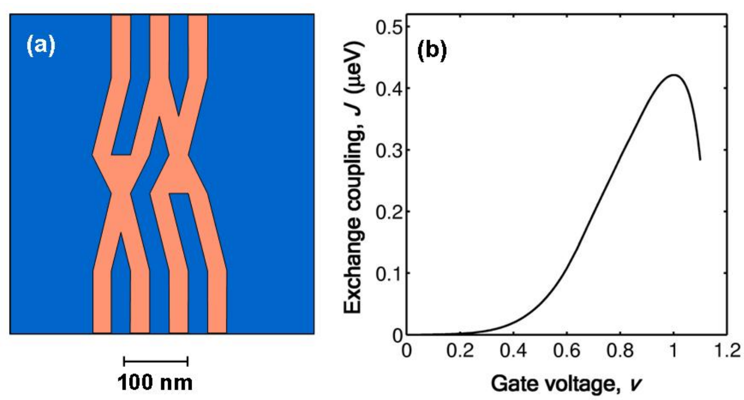

Fig. 13. Digital qubit architecture. **(a)** Top-gate structure for two qubits. **(b)** Simulation results for exchange coupling, J. J = maximum and $J = 0$ for the desired pseudo-digital working points, where J varies weakly with small voltage fluctuations, v.

towards one another along their axis, our design allows the electrons to slide *past* one another, in electrostatically defined "channels." At their closest approach, the electrons experience a maximum in their exchange coupling which provides a useful working point, Fig. 13 (b). We find that the pseudo-digital technique improves gate accuracy by *more than two orders of magnitude*. These simulations point to the feasibility of two-qubit gates for our proposed qubit architecture.

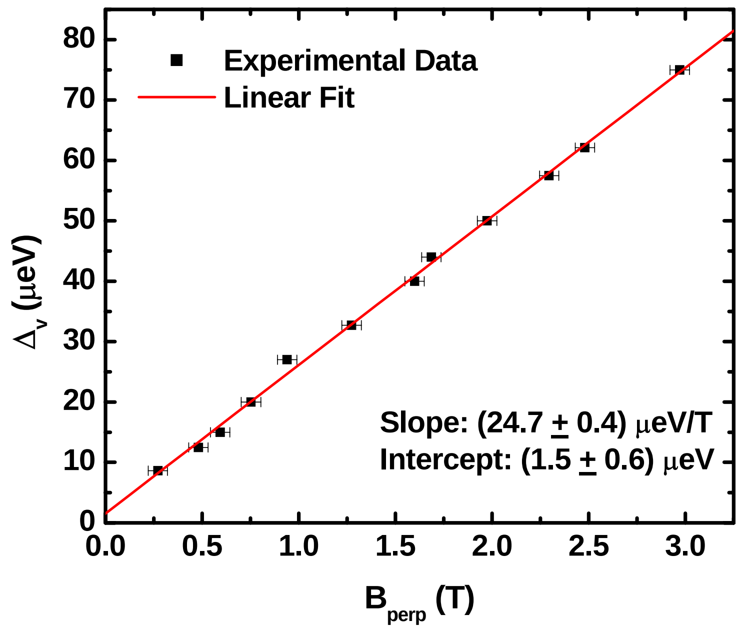

Fig. 14 Valley splitting as a function of applied magnetic field.

Bacon *et al.* [PRL 85, 1758 (2000)] and DiVincenzo et al. [Nature 408, 339 (2000)] have shown how *one*-qubit gates can be formed using the exchange interaction together with coded qubits. Thus, our pseudo-digital, back-gated qubit design has the potential to enable a complete set of gates for universal, fast and fault tolerant quantum gating.

9. Spectroscopy of valley splitting in silicon

In recent years several efforts have been made to study electron states in low dimensional systems. Due to the small number of spins and low-temperature requirements, conventional microwave absorption spectroscopy techniques (which require $10^{11} – 10^{12}$ spins for an appreciable resonance signal) are hard to employ in these structures. Transport measurements are the ideal way to probe such systems.

Bulk, unstrained silicon has six equivalent conduction band valleys. In strained silicon quantum wells, like those we discuss in throughout this report, this degeneracy is partially lifted by the strain, and only the two valleys along the <100> growth direction are relevant. This remaining degeneracy is split by quantum confinement, and perhaps by other mechanisms as well – this is an open question. We have shown that electronic transitions can be driven between these two lowest valley states in silicon using microwaves, ie. electron valley resonance (EVR). The valley splitting is found to increase linearly with applied perpendicular magnetic field (B_{perp}) – see Fig. 14. We were able to confirm this behavior over an order of magnitude in magnetic field. The ability to probe valley splitting with a microwave spectroscopy opens the possibility to engineer the valley splitting through changes in the underlying heterostructure – the focus of ongoing work.

(6)(a) Papers Published in Peer Reviewed Journals

- “Decoherence of electron spin qubits in Si-based quantum computers,” Charles Tahan, Mark Friesen, and Robert Joynt, Phys. Rev. B 66 035314 (2002).

- “Electrically Isolated SiGe Quantum Dots”, Emma Tevaarwerk, P. Rugheimer, O.M. Castellini, D.G. Keppel, S.T. Utley, D.E. Savage, M.G. Lagally, and M.A. Eriksson, Appl. Phys. Letters 80, 4626 (2002).

- “Pseudo-Digital Quantum Bits,” Mark Friesen, Robert Joynt, and M. A. Eriksson, *Appl. Phys. Lett*. **81**, 4619 (2002).

- “Strain Engineering, Self-Assembly, and Nanoarchitectures in Thin SiGe Films on Si”, A. R. Woll, P. Rugheimer, and M. G. Lagally, Materials Science & Engineering B96, 94 (2002).

- "Practical design and simulation of silicon-based quantum-dot qubits," Mark Friesen, Paul Rugheimer, Donald E. Savage, Max G. Lagally, Daniel W. van der Weide, Robert Joynt, and Mark A. Eriksson, *Phys. Rev. B Rapid Communications* **67**, 121301(R) (2003).

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- "Spin readout and initialization in a semiconductor quantum dot," M. Friesen, C. Tahan, R. Joynt, and M.A. Eriksson, *Physical Review Letters* **92**, 037901 (2004).

- “Coulomb Blockade in a Si:SiGe Two-Dimensional Electron Gas Quantum Dot,” L.J. Klein, K. Slinker, J.L. Truitt, S Goswami, K.L.M. Lewis, S.N. Coppersmith, D.W. van der Weide, Mark Friesen, R. Blick, D.E. Savage, M.G. Lagally, Charlie Tahan, Robert Joynt, M.A. Eriksson (University of Wisconsin Madison), J.O. Chu, J.A. Ott, P.M. Mooney (IBM Research Division, T. J. Watson Research Center), *Appl. Phys. Lett.* **84**, 4047-4049 (2004).

- "One-spin quantum logic gates from the exchange interaction and a global magnetic field," Lian-Ao Wu, Daniel A. Lidar, and Mark Friesen, Phys. Rev. Lett. **93**, 030501 (2004).

(6)(b) Conference Proceedings

- “Strain Relaxation in SiGe Thin Films Studied by Low-Energy Electron Microscopy”, A.R. Woll, P. Moran, E.M. Rehder, B. Yang, T.F. Keuch, and M.G. Lagally, Mat. Res. Soc. Symp. Proc. Vol. 696, N4.2 (2002).

- "Pseudo-Digital Qubits: A General Approach," M. Friesen, R. Joynt, and M. A. Eriksson, in Proceedings of the 6th International Conference on Quantum Communication, Measurement and Computing (QCMC02) (Rinton Press, Princeton, NJ, 2003), pp. 271-274.

(6) (c) Presentations at Meetings
"Modeling interactions of Si-Ge qubits," Mark Friesen, Mark Eriksson, R. Joynt,
M. G. Lagally, D. W. van der Weide, P. Rugheimer, and D. E. Savage, American Physical Society March Meeting, Seattle, WA, March 2001.

"Novel morphology and properties of 3D Ge islands grown on patterned Si-on-Insulator (SOI) substrates," P. Rugheimer, S.T. Utley, E.R. Tevaarwerk, D.E. Savage, M.A. Eriksson, P. Moran, T.F. Kuech, M.G. Lagally, and E. Mateeva, American Physical Society March Meeting, Seattle, WA, March 2001.

"Can quantum dot qubits work?" M. Friesen, P. Rugheimer, D. E. Savage, M. G. Lagally, D. van der Weide, R. Joynt, and M. A. Eriksson. International Conference on Quantum Information, Rochester, NY, June 2001. Poster

"Strain engineering, self-assembly, and nanoarchitectures in the SiGe system," A.R.Woll, P. Rugheimer, and M. G. Lagally, Sixth International Conference on Atomically Controlled Surfaces, Interfaces, and Nanostructures, Lake Tahoe, CA, July 2001. invited

"Electrical characterization of carrier confinement in Si/SiGe nanostructures", F. S. Flack, D. Savage, M. G. Lagally, K. Slinker, P. Rugheimer, M. A. Eriksson, Materials Research Society Fall Meeting, Boston, MA, November 2001. Poster

"Influence of gate voltage sequences and charged impurities on bound spins in small quantum dots", M. Friesen, P. Rugheimer, D.E. Savage, M.G. Lagally, D.W. van der Weide, Robert Joynt, and M.A. Eriksson. Materials Research Society Fall Meeting, Boston, MA, November 2001.

"Admittance spectroscopy of Si/SiGe nanostructures with p-type and n-type doping," K.A. Slinker, F.S. Flack, D.E. Savage, P. Rugheimer, M.A. Eriksson, M.G. Lagally, Y. Zhao, Materials Research Society Fall Meeting, Boston, MA, November 2001.

"Electrical characterization of carrier confinement and thermalization in Si/SiGe nanostructures," F.S. Flack, D.E. Savage, P. Rugheimer, K.A. Slinker, M.A. Eriksson, M.G. Lagally, Y. Zhao, Materials Research Society Fall Meeting, Boston, MA, November 2001.

"Heterogeneous electrical properties of SiGe nanostructures determined by electric force microscopy," E.R. Tevaarwerk, P. Rugheimer, D.E. Savage, M.G. Lagally, M.A. Eriksson, Materials Research Society Fall Meeting, Boston, MA, November 2001.

Fall MRS Meeting, December 2-6, 2002, Boston, MA, *Toward Spin Based Silicon-Germanium Quantum Dot Qubits*, K.A. Slinker, Mark Friesen, D.E. Savage, M.M. Roberts, M.G. Lagally, Robert Joynt, D.W. van der Weide, M.A. Eriksson, University of Wisconsin-Madison.

Fall MRS Meeting, December 2-6, 2002, Boston, MA, *Pseudo-Digital Quantum Bits*, Mark Friesen, Robert Joynt, and Mark A. Eriksson, Dept of Physics, University of Wisconsin.

Workshop on Solid State Quantum Computation, October 18-20, 2002 University of Illinois at Urbana-Champaign, *Towards silicon-germanium quantum dot qubits*, Mark Eriksson, Susan Coppersmith, Mark Friesen, Robert Joynt, Max Lagally, Michelle Roberts, Don Savage, Keith Slinker, Charles Tahan, Jim Truitt, and Daniel van der Weide, University of Wisconsin-Madison. (Poster)

Gordon Research Conference: Nanostructure Fabrication, August 4-9, 2002, Tilton School, Tilton, NH, *Pseudo-Digital Exchange Interaction for Solid-State Quantum Computation*, Mark Eriksson, Mark Friesen, Keith Slinker, Paul Rugheimer, Donald E. Savage, Max G. Lagally, Daniel W. van der Weide, Robert Joynt, University of Wisconsin-Madison. (Poster)

6th International Conference on Quantum Communication, Measurement and Computing (QCMC'02), July 22-26, 2002, Cambridge, Massachusetts, *Digital Qubits*, Mark Friesen, Robert Joynt, and Mark A. Eriksson (Poster).

Invited talk: QIS Short Course, May 27-31, 2002, Insbruck, Austria, *SiGe Quantum Dots: Pseudo-Digital Exchange?* Mark Friesen, University of Wisconsin-Madison.

Workshop on Quantum Device Technology, Clarkson University, Potsdam, New York, May 20–24, 2002, *A SiGe Quantum Dot Quantum Computer*, Mark Friesen, Keith Slinker, Paul Rugheimer, Donald E. Savage, Max G. Lagally, Daniel W. van der Weide, Robert Joynt, and Mark A. Eriksson, University of Wisconsin-Madison. (Poster)

Invited Talk: Solid-State Quantum Computation 2002, April 25, IBM Watson, *SiGe Quantum Dots: Pseudo-Digital Exchange?* Mark Eriksson, University of Wisconsin-Madison.

March Meeting of APS, Indianapolis, IN, March 18-22, 2002, *Designing Better Qubits*, Mark Friesen, Robert Joynt, M. A. Eriksson, University of Wisconsin-Madison.

March Meeting of APS, Indianapolis, IN, March 18-22, 2002, *Admittance Spectroscopy of Self-assembled Ge Quantum Dots and Wetting Layers on Si*, K.A. Slinker, F.S. Flack, D.E. Savage, P. Rugheimer, M.G. Lagally, M.A. Eriksson, University of Wisconsin-Madison.

"Quantum Computing using SiGe Quantum Dots"
Invited Paper at the International Workshop on Correlated Electrons and Emergent Phenomena, International Center for Theoretical Physics, Trieste, Italy, August, 2002 (presented by R. Joynt)

"Quantum Random Walks," Paper at the ERATO Workshop on Quantum Information, University of Tokyo, Tokyo, Japan, September, 2002 (presented by R. Joynt)

"Quantum Computing using SiGe Quantum Dots"
Invited Paper at International Workshop on Physical Implementations of Quantum Computing, Osaka, Japan, September, 2002 (presented by R. Joynt)

Niels Bohr Summer Institute on Complexity and Criticality, Copenhagen, August 2003, Susan Coppersmith.

Solid State Quantum Information Processing Conference, Amsterdam, The Netherlands, December 18, 2003, “Silicon-germanium quantum dots for quantum computation,” Mark A. Eriksson.

Workshop on Group-IV Quantum Computing, March 29, 2003, “Gated Si:SiGe quantum dots for quantum computation,” Mark A. Eriksson.

APS March Meeting, March 2003, “Towards few electron silicon-germanium quantum dots: progress and challenges,” Mark A. Eriksson.

"Gating and Readout of Spin Qubits in Silicon Quantum Dots," by Mark Friesen, Workshop on Computational Approaches Towards the Electronic Properties of Quantum Dots, Chicago, IL, 09/24/03.

"Spin Read-out and Initialization in a Silicon-Germanium Quantum Dot Qubit," by Mark Friesen, Charles Tahan, K. A. Slinker, Levente J. Klein, D. W. van der Weide, Robert Joynt, and M. A. Eriksson, contributed talk at the Materials Research Society Spring Meeting, San Francisco, CA 04/23/03.

"Quantum Dot Spin Readout and Initialization by Microwave Excitation," by Mark Friesen, Charles Tahan, Robert Joynt, and M. A. Eriksson, poster presentation at the Gordon Conference on Quantum Information Processing, Ventura, CA , 03/25/03.

Solid State Quantum Information Processing Conference, December 15-18, 2003, Amsterdam, The Netherlands, *SiGe quantum dots for Quantum Computation*, L.J. Klein[1], K. Slinker[1], J. Truitt[1], S. Goswami[1], K. Lewis[1], S. Coppersmith[1], D. van der Weide[1], M. Friesen[1], R. Blick[1], D. Savage[1], M. Lagally[1], C. Tahan[1], R. Joynt[1], J.O. Chu[2], J.A. Ott[2], M.A. Eriksson[1], [1]University of Wisconsin-Madison, [2]IBM-Watson (Poster).

Directed Assembly, Strain Engineering, and Materials Integration on Silicon, M.G. Lagally, MRS Meeting Dec 03 Boston

Nanoscience and Technology on Silicon: Directed Assembly, Strain Engineering, and Materials Integration, M.G. Lagally, ACSIN 7, Nara, Japan, Nov 03

"The role of impurities in quantum dot quantum computers," by Shaolin Liao, M. A. Eriksson, and Mark Friesen, Poster presentation at the American Physical Society March Meeting, 2003, San Antonio, TX, 03/04/03.

"A SiGe Quantum Dot Quantum Computer," Keith Slinker, Levente Klein, Mark Friesen, Jim Truitt, Donald E. Savage, Max G. Lagally, Daniel W. van der Weide, Robert Joynt, and Mark A. Eriksson, poster presentation at the Gordon Conference on Quantum Information Processing,Ventura, CA , 03/25/03.

APS March Meeting, 2003, *Silicon-Germanium Nanostructures for Quantum Dot Qubits*, K.A. Slinker, Friesen Mark, L.J. Klein, D.E. Savage, K.L. Morgenstern, A.M. Petrowski, M.M. Roberts, M.G. Lagally, Robert Joynt, D.W. van der Weide, M.A. Eriksson, University of Wisconsin-Madison.

Gordon Research Conference on Quantum Information Science, March 2003, Ventura, CA, *Strained silicon quantum wells for quantum information and quantum computing*, K.A. Slinker, L. Klein, Mark Friesen, D.E. Savage, M.M. Roberts, M.G. Lagally, Robert Joynt, Dan van der Weide, and M.A. Eriksson, University of Wisconsin-Madison (Poster).

Conference Poster: December 15-18, 2003: "Signatures of silicon: Spin and valley states in SiGe quantum wells," Solid State Quantum Information Processing Conference, Amsterdam, The Netherlands, C. Tahan, et al.

Conference Talk: August 9, 2003; "Spin Readout and Initialization in a Semiconductor Quantum Dot," 2nd International Workshop on Quantum Dots for Quantum Computing and Classical Size Effects Circuits, Notre Dame, IN, C. Tahan, et al.

Conference Talk: March 7, 2003; "Single Qubit Spin Readout and Initialization in a Quantum Dot Quantum Computer: Design and Simulation," APS March Meeting (Austin, TX), C. Tahan, et al.

March 28, 2004; "Spin and pseudo-spin states in silicon for QC: lifetimes," APS March Meeting (Montreal, CA), C. Tahan, et al.

"Three Quantum Dots Embedded in Aharonov-Bohm Rings," APS March Meeting 2004 Session B37: Spin Qubits and Quantum Dots. Monday Midday, 26 March 2004, Ryan Toonen, Andreas Huettel, Srijit Goswami, Karl Eberl, Mark Eriksson, Daniel van der Weide, Robert Blick

"Etched Devices for Silicon Quantum Computing," at 2004 IEEE NTC Quantum Device Technology Workshop, Clarkson University, Potsdam, New York, May 17-21, 2004.

(6)(d) Manuscripts submitted but not yet published

- "Spectroscopy of Valley Splitting in a Silicon/Silicon-Germanium Two-Dimensional Electron Gas," Srijit Goswami, J. L. Truitt, Charles Tahan, L. J. Klein, K. A. Slinker, D. W. van der Weide, S. N. Coppersmith, Robert Joynt, R. H. Blick, Mark A. Eriksson, J. O. Chu, P. M. Mooney, cond-mat/0408389, submitted to *Phys. Rev. Lett*.

- "Rashba spin-orbit coupling and spin relaxation in silicon quantum wells," C. Tahan and R. Joynt, accepted for publication in *Phys. Rev. B* (2003)

- Timothy B. Boykin, Gerhard Klimeck, Mark Friesen, S.N. Coppersmith, Paul von Allmen, Fabiano Oyafuso and Seungwon Lee, "Analytic solution methods for tight-binding models of quantum-confined heterostructures," accepted by Physical Review B.

- M. Prada, R.C. Toonen, R.H. Blick and P. Harrison, "Electron-Nuclear Spin Transfer in Quantum Dot Networks" submitted to IOP.

7. Scientific Personnel Supported and Advanced Degrees Earned

Name	Title	Degrees Received
ERIKSSON, MARK A	faculty	
JOYNT, ROBERT J	faculty	
VANDERWEIDE, DANIEL	faculty	
BRACE, CHRIS L	grad	
GOSWAMI, SRIJIT	grad	
RUGHEIMER, PAUL	grad	Ph.D.
SLINKER, KEITH A	grad	
TAHAN, CHARLES G	grad	
TRUITT, JAMES L	grad	Passed Ph.D. Defense - Degree in Dec. 2004
ZHANG, PENGPENG	grad	
FLACK, FRANK S	postdoc	
KLEIN, LEVENTE I	postdoc	
FRIESEN, MARK G	scientist	
LIMBACH, STEVE	scientist	
SAVAGE, DONALD E	scientist	
BHOOT, DHRUV SURESH	undergrad	
LEWIS, KRISTIN L	undergrad	
PETROWSKI, ALANE	undergrad	
ZEPPENFELD, MARTIN G	undergrad	

8. Inventions

- Spin-Bus for Spintronic Information Transfer: A Spin Chain of Strongly-Coupled Quantum Dots

- A Self-Contained, Patterned Quantum DOT Devise for Spin to Charge Transduction, Readout and Initialization, for use in Quantum Computing and Quantum Information Processing

- Solid-State Qubits Combinning Surface Gates with Tunnel-Back-Gates